

Durham Research Online

Deposited in DRO:

07 March 2017

Version of attached file:

Accepted Version

Peer-review status of attached file:

Peer-reviewed

Citation for published item:

Clark, S.J. and Lancaster, T. (2017) 'The use of downward causation in condensed matter physics.', in Philosophical and scientific perspectives on downward causation. New York: Routledge, pp. 131-145. Routledge studies in contemporary philosophy. (91).

Further information on publisher's website:

<https://www.routledge.com/9781138195059>

Publisher's copyright statement:

This is an Accepted Manuscript of a book chapter published by Routledge in Philosophical and Scientific Perspectives on Downward Causation on 24/02/2017, available online: <http://www.routledge.com/9781138195059>

Additional information:

Use policy

The full-text may be used and/or reproduced, and given to third parties in any format or medium, without prior permission or charge, for personal research or study, educational, or not-for-profit purposes provided that:

- a full bibliographic reference is made to the original source
- a [link](#) is made to the metadata record in DRO
- the full-text is not changed in any way

The full-text must not be sold in any format or medium without the formal permission of the copyright holders.

Please consult the [full DRO policy](#) for further details.

The use of downward causation in condensed matter physics

Stewart J. Clark and Tom Lancaster
Department of Physics, University of Durham, South Road,
Durham DH1 3LE, UK

July 17, 2016

1 Introduction

When atoms are brought together to form a solid, electrons interact quantum mechanically and new states of matter emerge. These include ordered states, new excitations and unusual “topological” objects [1, 2]. Modern condensed matter physics is the investigation of this exotic, emergent world of quantum matter and provides an insight into the Universe just as fundamental as the study of elementary particles or black holes. Downward causation is invoked less in physics than in the philosophy of physics, although in the debate surrounding emergence it is often raised as a possible explanation for the condensation of complex states of aggregative matter [3].

In the context of condensed matter physics, an explanation based on downward causation might be framed as follows: microscopic constituents of matter interact at a lower level quantum mechanically via a relatively simple set of interactions, such as the Coulomb repulsion of similarly charged electrons in the presence of the oppositely charged atomic nuclei. It is, at present (at the very least), an impossible task to follow the details of all of these interactions and their consequences, because in a macroscopic sample (say, a gram or so in weight) it would typically involve keeping track of $N \approx 10^{23}$ particles and their pairwise interactions with all of the other particles. However, it is often found that the behaviour of the system can be well described by variables that result from averaging over the behaviour of fine-grained degrees of freedom such as the particles’ momenta or magnetic moments.¹ This so-called *course-graining* routine of averaging over degrees of freedom that change fairly slowly in space and time results in the macroscopically defined variables operating at a higher level. (A more technical definition of course graining is replacement of microscopic degrees of freedom by average variables on an expanded length scale [2].) This leads to the consideration of two levels of behaviour: the lower, microscopic

¹For example, temperature is a measure of the average kinetic energy of the particles that constitute the system.

level at which electrons operate and the upper, macroscopic level, operating on an expanded length scale, at which we make many of our measurements. In physics, the coarse grained variables are often viewed as causally interacting downwards on individual microscopic constituents of the matter. This may be described in terms of providing boundary conditions or constraints (such as the walls of a container containing the atoms of a gas) or more directly (such as the effective field theories described below). This is the *physics* of downward causation and we examine it in this essay, giving several examples from the field of condensed matter physics.

The general theme of our examples is as follows: calculating the properties of a macroscopic system often involves coupling a microscopic subsystem with a macroscopic reservoir, and this result in fields or other boundary conditions that dictate behaviour. By identifying this as downward causation we are, in the sense stressed by Blundell [4], tracing out a causal path for our own convenience in describing and understanding the complex behaviour of many-particle systems. Moreover, we shall see below that the causal links we find are more complicated than those that would simply imply a top-down process. However, with this in mind, we believe that the scheme that we describe here, which does not invoke any mysterious higher level physics, does cast light on the use and limitations of notions of downwards causation in physics, particularly in the emergence debate.

Below we describe in detail some common examples of how these ideas are applied where we discuss their use in identifying novel behaviour in condensed matter, their shortcomings and their place in a hierarchical series of approximations known as a perturbation series. We then turn to density functional theory, which is a first principles method of describing real systems of condensed matter, whose practical implementation involves many concepts involved in the discussion of downwards causation.

2 Mean field theory

The sketched description of downward causation given above is very similar to the description of a much-used technique in theoretical physics: *mean field theory*. Mean field theory is most easily explained in terms of a simple-minded picture of a magnet. This is formed from magnetic moments (or *spins*) s_i positioned at points labelled i on a regular lattice. (For our purposes we adopt the *Ising model* where the spins can be constrained to take only two possible values $s = \pm 1$, i.e. they align or anti-align along a single direction.) The energy of a microscopic moment in an applied magnetic field B is given by $E_i \propto s_i B$. Moments will also have a microscopic interaction with their neighbours, usually this is of the Heisenberg form $-Js_1s_2$. This means that for pairs of magnetic moments there is an energy contribution that depends on whether the neighbouring spins are aligned or anti-aligned. This represents a complete microscopic description of the physics of the components of this model magnet.

Turning to a large system of N interacting spins and following the usual

rules of statistical physics, we may write an expression for the expected value of spin at site i at temperature β , which turns out to be given by

$$\langle s_i \rangle = -\tanh \left[\beta \left(J \sum_j s_j - B \right) \right], \quad (1)$$

which, in words, says that a spin sits in the *effective field* (the part in braces in the above equation) formed from the applied field B and the spin exchange field of its neighbours [5]. To get the true value of $\langle s_i \rangle$ we must average over all values that the neighbouring spins s_j can take. The weight for these involves the interaction of these spins with their own neighbours and so on. This is a serious problem in that, for the usual case of $N \approx 10^{23}$ spins in a typical macroscopic solid, such a computation is, at best, impractical. To break this ladder of successively more complicated interactions we make the *approximation* that the effective field is changed from $(B - J \sum_j s_j)$ to $(B - Jz\langle s \rangle)$, where $\langle s \rangle$ is the average spin and z the number of interacting neighbours of the spin s_i . This effective field is most naturally expressed at the macroscopic level, where we introduce a course-grained variable $M = \frac{1}{V} \sum_i s_i = n\langle s \rangle$, where $n = N/V$ and V is the volume of the solid. *This is where the downward causation comes in.* We ask what causes the magnetic field on a particular microscopic spin s_i at position i . We answer that it is the field B we apply, plus the effective field caused by the magnetization in its vicinity which reflects the average behaviour of aligned local spins. Notice the circularity of the argument: (i) what causes the spin at a particular microscopic site to align is the (high level) magnetization field at that spin site; (ii) what causes the average magnetic moment (i.e. the magnetization) is the fact that lower level spins are aligned.

What new information does such an approach reveal? To see most clearly the novel consequence of introducing the effective field we replay the above statistical argument in the language of thermodynamics. This is done through examining the magnetic susceptibility χ , which is a measure of how easily the magnetisation of a material changes for a given applied magnetic field. Consider first a paramagnet: a system without internal interactions (i.e. one with $J = 0$), merely a collection of isolated spins subject only to an applied field B . When such a paramagnetic system is subject to a magnetic field its magnetization changes according to

$$\mu_0 M = \chi B, \quad (2)$$

where μ_0 is a constant and χ is the magnetic susceptibility: the response of the system to an external stimulus. That is to say that the magnetization M is caused by any applied field lining up the spins. (Since there are no interactions, this is the only thing that can happen.) Pierre Curie discovered that the randomizing influence of temperature T makes a paramagnet less susceptible to being magnetized, such that $\chi = C/T$, where C is a constant. This allows us to say $\mu_0 M T = C B$. Now we turn the interactions back on. Assuming M is constant across the system, we reintroduce our effective field by replacing

$B \rightarrow B + \mu_0 \lambda M$. What causes the additional term, $\mu_0 \lambda M$, in the effective field? As in the statistical case above, it is the interactions between the microscopic spins, which we have reintroduced into the system in a top-down manner with this move. We find

$$\mu_0 M T = C(B + \mu_0 \lambda M), \quad (3)$$

and solving for M we have

$$\chi = \frac{\mu_0 M}{B} = \frac{C}{T - \lambda C}. \quad (4)$$

The result of these manipulations is that the expression for χ diverges (when the denominator in the above expression becomes zero) at some value of T given by $T = T_c = \lambda C$. This corresponds to a *ferromagnetic transition*: the spins spontaneously align with each other such that we get magnetization M in the absence of an applied field. This is a novel property of the system that is predicted by the mean field approximation.

Summarising the above result, we introduced an effective field via a macroscopic variable M which causes a novel feature in the behaviour of the system: the magnetic ordering of the microscopic spins. A single, lower level, microscopic spin is influenced by the collective behaviour of its neighbours, which acts downwards from the higher level to cause the microscopic spins to align. It is worth stressing that the circularity of the argument shows that the causal path involved in mean field theories is more subtle would be implied by describing it as “top-down”.

In the next section we will see how this argument pervades the subject of solid state physics.

3 The electron gas

The mean field model is used in many contexts, but perhaps the most well-studied is the metal [6], where electrons are free to move throughout a macroscopic sample of material. The physics of metals has been called the equivalent of the standard model of condensed matter physics [6]. Here we describe an idealized model of the metal known as the electron gas, before turning to real materials in Section 4.

A metal may be thought of as a box containing electrons that each carry a charge e . But we want the system to be electrically neutral (no net charge) and so we have to introduce positive charge into the system. In a real material this would be the charge associated with atomic nuclei. However in the model system we describe here, we instead imagine the box also contains sufficient positive charge to make the overall system electrically neutral (which is spread evenly throughout the box) to form a stable state of matter. Electrons being indistinguishable Fermions means that they must obey the Pauli exclusion principle: no two may share the same quantum numbers. If we imagine building a metal by adding electrons to the box, then Pauli exclusion forces us to put

two electrons in the lowest energy level (the fact that electrons carry a spin quantum number taking two possible values explains why each energy level may accommodate exactly two electrons), then next two in the next lowest and so on. The consequence is that the electrons stack up in energy, with the highest energy level (the so-called Fermi energy) being so energetic that the electron has sufficient energy to travel at some 10^6 ms^{-1} : a remarkably high speed.

From a microscopic point of view the physics of the metal is determined by the sum of the energies of the electrons. This is formed from a kinetic energy part (which turns out to be exactly that part described in the previous paragraph) and a potential energy part. The potential energy is simply that due to the Coulomb repulsion of the electronic charges

$$V = \sum_i \frac{e^2}{4\pi\epsilon_0 x_i}, \quad (5)$$

where x_i is the separation of the electrons and the sum is over all pairs. Despite being very simple, the resulting model of a metal does not admit an exact solution. As in the magnetic case, we again invoke a mean field approximation. As we will discuss below, the mean field approximation actually provides the first term in a perturbation series that provides a highly successful but necessarily approximate solution to the behaviour of the metal, closely akin to the description of electrons and photons in quantum electrodynamics[6].

The result of invoking the mean field approximation to the metal is that the potential energy falls apart into two terms known as (i) the Hartree term and (ii) the Fock term. Each of these describes a process of an individual electron being interacted upon via a coarse-grained variable $\sum_k \langle n_k \rangle$ that reflects the collective, higher level action of the other electrons in the system. In this case the effective field $\sum_k \langle n_k \rangle$ is simply the number of interacting electrons. Moreover, the two terms may be interpreted as causal processes which individual electrons undergo. (i) The Hartree term describes an electron that interacts with all of the electrons in the system by creating another excited electron, that immediately drops back to its original state of energy. (ii) The Fock term describes an electron that creates another excited electron and then fills the empty state just vacated. The excited electron then takes the place of the original one.

A key idea in this sort of theory (known as many-body physics) is the concept of renormalization. This may be thought of as the process that determines how the system (taken as the sum of constituents plus their interactions) changes the properties of the constituents themselves. In the case of the metal, the constituents are individual electrons and the result of the interactions of the system their properties change: specifically their masses and charges take different values to those of a free electron (we will discuss this in more detail, below). The particles that make up the system can therefore be very different quantitatively (and even qualitatively) from their values in the absence of the interacting system. To reflect this, they are often called *quasiparticles*. Conceptually a quasiparticle may be thought of as

$$(\text{quasiparticle}) = (\text{bare particle}) + (\text{interactions}). \quad (6)$$

One goal of many-body physics is to explain the corrections to the properties of the bare particle that we notice when comparing it to the particle inside the system. We note that although the pseudo-equation above appears to conflate single particle and collective descriptions, Landau's adiabatic continuity argument [7] shows that bare particles and quasiparticles that belonging to the same thermodynamic phase are in a one-to-one correspondence.

This is the content of a mean field theory of a metal, this one being known as the Hartree-Fock theory, for obvious reasons. It provides us with an estimate for properties of the metallic state of matter (including the energy). However, it gets a lot of properties wrong: in particular the mass of the highest energy ground state electrons, which it predicts to be zero. This is clearly incorrect: the mass of electrons in a metal is usually of the same order as the bare electron mass in the vacuum.

So this mean field theory is not a good basis alone for understanding the metal² and provides no qualitatively new information. In order to improve the mean field result and to reveal new phenomena, it is necessary to consider it as the first stage in a ladder of corrections to the properties of the bare particle. This is formalised into a method known as a *perturbation theory* in which the terms are arranged in order of the number of interactions an electron has with the system. (For the mean field description the electrons interact only once.)

Going beyond the mean field result reveals a new class of interactions known collectively as *correlations*. The most relevant type of these interactions in the electron gas is a little like a more complicated version of the Fock term described above. This type involves an electron being ejected from below the Fermi level and then, a little later, meeting up with the empty state left behind. Considering the effect of all such possible interactions of this sort in the system results in the so-called *Random Phase Approximation* (RPA). The RPA not only gives us a correction to the mean field result that provides a good estimate of the electron mass, it also reveals a new phenomenon: an excitation of the whole of the metal known as the plasma oscillation. This excitation, invisible to the theory of mean fields involves all of the electrons acting together to shift back and forth in space with respect to the positively charged background. The plasma oscillation was predicted by Bohm and Pines [8] and, historically, was the first predictive triumph of many-body theory: plasma oscillations were later measured experimentally.

The moral of this story is that the sort of downward causation that the physicist routinely invokes is only a crude approximation to reality. However it is valuable in that it is, formally speaking, the first order correction to a perturbative series that approximates reality very closely. Further approximations are often necessary to reveal new physics.

²Although we note that a reformulated mean field theory proposed recently been shown to describe some simple metals accurately.

4 First principles calculations

Let us now move away from highly idealized model condensed matter systems and turn our attention to a method of calculating the properties of real materials from first principles. Despite the large number of particles in a condensed matter system, we are able to write down the equations governing the constituents (i.e. the nuclei and electrons) from which, in principle, that all other properties can be derived. The result is the N -particle Schrödinger equation of the system. To be explicit, if we have N quantum particles at positions r_1, r_2, \dots, r_N then the wavefunction of this system is a function of all of these co-ordinates $\Psi(r_1, r_2, \dots, r_N)$. As noted above, for a condensed matter system N is approximately 10^{23} for a few cubic millimeters of material. All of the electrostatic interactions (which give the potential energy) between all pairs of particles can be written down using Coulomb's law and the kinetic energy relating to the momentum of the particles also has a particularly simple mathematical form. If we let the symbol H represent these energy contributions (H is known as the Hamiltonian of the system) then the N -particle Schrödinger equation is

$$H\Psi(r_1, r_2, \dots, r_N) = E\Psi(r_1, r_2, \dots, r_N) \quad (7)$$

where E is the energy of the system. There is also a variant of this equation which gives us time-dependency, but for our illustrative purposes here we do not need that detail. This equation has many solutions with discrete energies: the solution with the lowest energy is known as the ground state, and higher energy states known as excited states. It was with this equation in mind (along with its time-dependent and relativistic forms) that Dirac made the remark [9]

The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble.

By that he meant if one could solve the N -particle Schrödinger equation for something (e.g. an atom, a molecule, assemblies of atoms in solids or liquids) one should be able to predict every physical property; this is more than a statement of empirical observation, Dirac implies (and many physicists would claim) that all of the physics required to determine the properties of materials is encompassed by this equation. This is what we mean by a *first principles* approach. It is vastly ambitious because its goal is to model real systems using no approximations whatsoever. However, Dirac continues:

It therefore becomes desirable that approximate practical methods of applying quantum mechanics should be developed, which can lead to an explanation of the main features of complex atomic systems without too much computation.

It has taken great effort and ingenuity to bring us to the point where such a method, *density functional theory*, has been formulated which gives us access to accurate densities and energies that now allows us to calculate *some* of the properties of materials from first principles. Density functional theory is a form of mean field theory that has proven the most successful method of addressing the N -particle quantum problem in condensed matter systems [11, 12]. It is both a profound, exact theory for interacting electrons, and a practical prescription for calculating exact or approximate values of the systems properties. The beauty of DFT is that one makes no attempt to compute the N -particle wavefunction itself, but instead aims to calculate the *electron density*, that is, the probability of finding an electron at a particular point in space. This in itself is a quantity averaged over $N - 1$ of the degrees of freedom of the N -particle wavefunction. It therefore appears (in a mathematically exact sense) that, within density functional theory, $N - 1$ degrees of freedom of the wavefunction are not necessary for obtaining the properties of a material. We believe that this is an important statement in its own right.

Before examining density functional theory more closely, it is first necessary to examine what is meant by a N -particle quantum system. In quantum mechanics, we have one wavefunction that describes the entire N -particle system. We do *not* have N 1-particle wavefunctions. In fact, as soon as one speaks of the individual particles that the N -particle system contains, then it is usually the case that an approximation has been made, both conceptually and mathematically. An example is the discussion above where we treated bare particles and their interactions via a simple mean field approximation. There we approximate the form of the interactions. In other cases where we include an external influence such as an applied magnetic field, then we have implicitly divided our single system into ‘internal’ and ‘external’ parts. At that point an approximation is made, as we have subdivided a single N -particle wavefunction into an external wavefunction and internal wavefunction. No statement is usually made about the interaction between these two systems. In such simplifications, which have the general form of the division of the ‘material of interest’ from the ‘rest of the Universe’, we can write the influence of the ‘rest of the Universe’ as a boundary condition to our system, which can often be described by mathematically as ‘the application of an external field’. For first principles problems, therefore, it is this division which imposes the necessary conditions for the simplified form of downward causation we have described above.

An alternative description of the process outlined in the previous paragraph would be to consider a thermodynamically closed quantum system and then to focus on one open part of it. The influence of the rest of the system (i.e. the environment) on the open subsystem of interest can be described by macroscopic variables, such as fields. The result is two alternative ways to deal with a complex quantum system: (i) describe the closed system by finding its complete solution or (ii) to study an open subsystem of the whole system, under the influence of the environment that (in the classical limit) takes the form of a field. Although (i) is impractical and many cases and (ii) often involved an approximation, these two approaches were recently shown to be equivalent for

an example many-body quantum system [10].

Once we have our isolated system plus boundary conditions, we might ask what sort of properties can be mathematically derived using quantum mechanics. The answer, perhaps unsurprisingly, is those which can be expressed in a quantum mechanical manner. Consider the question “What colour is a material?” Although we are asking about a macroscopic property of a material, to answer the question from the Schrödinger equation we must reformulate the question in the language of quantum mechanics. If we shine white light onto a material, the light consists of a mixture of photons having wavelength in the visible region of the electromagnetic spectrum. If the difference in energy of the electron states in the material (the values of energy determined from the Schrödinger equation) approximately equals the energy of a photon then the photon will be absorbed by the material, otherwise it will be reflected/transmitted. The energy and hence wavelength of the unabsorbed photons gives us the colour of the material.

5 Density functional theory

We now turn to the nature of quantum condensed matter systems from the viewpoint of density functional theory, which is best thought of as an exact reformulation of the Schrödinger equation in a manner amenable to approximate solution.

Take an N -particle system where the electrons have a neutralising positive background (for example given by the positive charge on atomic nuclei). We can write exactly the Schrödinger equation of this system by considering the electron-electron Coulomb interaction and shown schematically in Figure 1 (left panel). It is not possible to solve the general N -particle Schrödinger equation analytically since the huge numbers of particles involved make it too computationally demanding, even with the current generation of supercomputers. However, we can get around this limitation with density functional theory. It may be shown mathematically that the total energy of a system including that of the many body effects of electrons in the presence of an external potential (for example, the atomic nuclei) is a unique functional of the charge density. As a result, the many-body quantum problem can be reformulated in terms of the charge density rather than the wavefunction.

If we denote the charge density of a system by $n(r)$ then the immediate reduction in dimensionality is obvious compared to the wavefunction $\Psi(r_1, r_2, \dots, r_N)$. The importance of being able to solve the N -particle quantum problem in terms of charge density rather than the wavefunction cannot be overstated. The dimensionality of the N -particle wavefunction is $3N$ (in 3 dimensions) but the dimensionality of the charge density is simply 3. Therefore all of the physical properties that can be extracted out of the $3N$ -dimensional wavefunction are folded up into the very much reduced dimensionality of the charge density. Note that it is not possible to reconstruct the N -particle wavefunction from the charge density; the reduction in dimensionality of the system is a one way

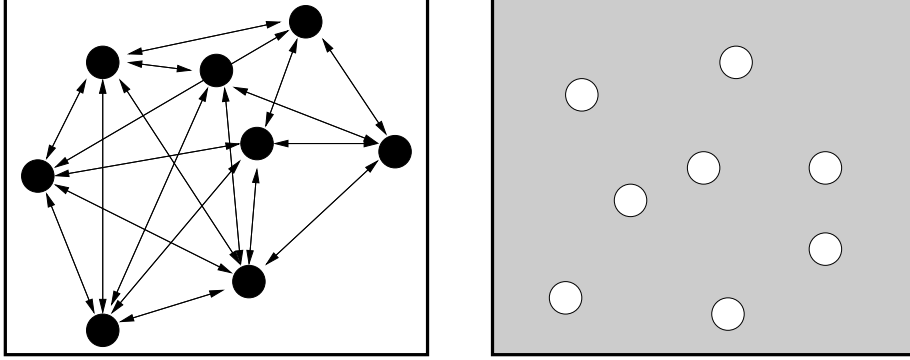


Figure 1: (Left panel): The electrons are shown schematically by black circles and the Coulomb interaction between some electrons are shown by arrows. (Right panel): a mean field DFT approach is shown where the DFT quasiparticles are shown by white circles swimming in a background field generated by the electric field of other particles.

process. In order to solve the resulting problem, we note finally that there is a Schrödinger-like equation associated with density functional theory

$$H[n(r)] = E[n(r)], \quad (8)$$

where we again obtain multiple solutions for the energy analogous to the Schrödinger equation.

Density functional theory clearly simplifies the many-body problem. However, the N -particle complexity of the quantum system is packaged up in contributions known as *exchange* and *correlation*. Roughly speaking, exchange is the (often sizeable) contribution to the energy from processes that generalize the Fock contribution described in Section 3. Correlation, alluded to above, is all the rest of the many-body processes that make a contribution. We give a more physical demonstration of the physical role of exchange in density functional theory in the next section. From a technical point of view, the exact form of the exchange and correlation contribution is, to date, unknown and is approximated in all practical calculations[13, 14, 15]. However, the fact that the unknown contribution is a functional of the charge density rather than the N -particle wavefunction is mathematically proven. Our discussion from here does not require the exact form, only the principle that we know that we are allowed to express exchange and correlation in terms of the charge density.

6 Exchange, correlation and the emergence of quasiparticles in DFT

To give an indication of what exchange and correlation represent physically, as well as to see what new information this approach reveals, we examine the

effect that they have on the charge density of the system in DFT. Exchange may be thought of physically as reflecting a mixture of electrostatic repulsion and the Pauli exclusion principle (i.e. that no two electrons can be in the same quantum state). If we consider a single electron in the system then the effect of exchange is to repel electrons from its vicinity. That is, it creates a *hole* for itself in the charge density. In fact, it can be shown that the volume of the hole that it creates around itself is exactly one electronic charge of opposite sign. An example of an exchange-hole is shown in Figure 2. Adding on correlation (i.e. all of the other contributions) to this gives a slight modification to the shape of the hole but does not change its volume.

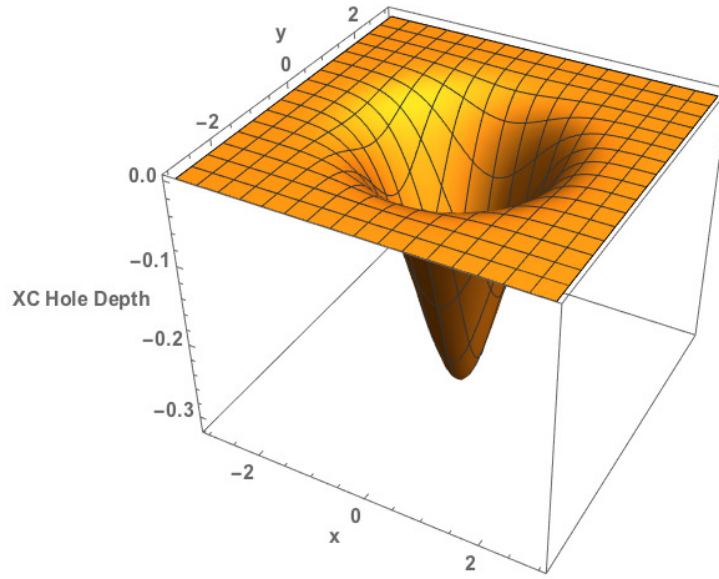


Figure 2: A representation of an exchange hole is shown in two dimensions (x and y axes are on the horizontal plane) while the depth of the exchange hole is given by the vertical axis. The volume of the hole is -1 in units of electron charge.

At this point we see that density functional theory has led us to the emergence of a new particle; the quasiparticle of the N -particle system (see section 3). The positively charged exchange-correlation-hole follows the electron around the system. They cannot be separated. Therefore to discuss electronic behaviour in terms of electrons and exchange-correlation holes is not a useful way to examine the N -particle quantum system. The quasiparticle consisting of electron plus exchange-correlation hole is now the most economical object that can be used explain the physics [Figure 1 (right)]. These quasiparticles have emerged from the system but do not exist as individual entities from which we fundamentally construct the system. The quasiparticles have unusual properties that

do not correspond to the properties of individual electrons. They are neutral (zero charge) particles and hence weakly interacting with each other from an electrostatic point of view. Moreover, by Newton's Second Law ($F = ma$) the acceleration of a particle is in the same direction as the force applied if its mass is positive. However, the quasiparticles of our system can accelerate counter to the force, and hence can be described as having a negative mass.

In fact, quasiparticles analogous to those we have described here are invoked in a number of different condensed matter systems where, it could be argued, they are treated metaphysically seriously. A well known example is the *hole* in semiconductor physics. Semiconductors are materials doped with atoms containing either one too few or one too many electrons to bond normally to neighbouring atoms. In the case of having one electron too few, then instead of focusing attention on the $N - 1$ electrons in the nominal N electron system, we examine the “ -1 ” electron in the system: the hole that is left. This hole behaves just like a real particle, it can have a mass and charge associated with it. However, one can doubt its existence in that it may also be described in terms of the $N - 1$ electrons acting in unison to give the appearance of the new particle. Such a hole is a quasiparticle of the semiconductor system, similar to the exchange-hole.

From the insight into exchange and correlation that the quasiparticle concept allows, we may finally elucidate the link between density functional theory and mean field theory. Density functional theory is actually a form of mean field theory, but there are differences to the simple form described in section 2. A mean field theory usually attempts to describe the actual particles from which that a system is constituted as moving in the *mean field* of the other particles, rather than following the exact prescription of summing over all possible particle-particle interactions. In density functional theory, the exact link between the density functional method and solving the Schrödinger equation is that both methods produce the same density of particles, that is, they both produce the same mean field. It is in this sense density functional theory is a mean field theory. However in density functional theory the particles of the system are not taken to be the constituent particles, but instead the weakly interacting quasiparticles (the electron plus its exchange and correlation hole in our example). The concept of a bare, constituent particle in density functional theory makes little physical sense. Given that the electron density is the object from which material properties can be derived, the mean field itself can be considered to be the most relevant physical object, rather than the constituent bare particles plus interactions.

7 Conclusions

A form of downwards causation is often invoked in mathematical physics, particularly in the context of condensed matter. This is the mean field model. In a general sense, the mean field model viewed as an approximation allows the prediction of novel phenomena such as the ordering at phase transitions. It can

also be viewed as the first stage in a hierarchical perturbation series, where the approximations that go beyond mean field theory can themselves reveal novel phenomena.

In condensed matter physics, one of the most useful tools based on this approach is density functional theory. This is a rather special form of mean field theory, whose first-principles nature allow us an insight into how boundary conditions arise, which can be thought of as a form of downward causation, and in this case leads to the emergence of a new form of particle in the system.

Finally we note that in the form of downward causation we have described, no mysterious extra physics is invoked to explain the workings of materials nor the emergence of novel properties and entities. Rather the novelty springs from two possible sources: the imposition of particular boundary conditions and the special forms of approximation invoked. Although this might make our account of downwards causation in condensed matter physics appear as a rather weak and epistemic notion, it is not weak in its explanatory power and there is no denying the effectiveness of mean field theory in modern condensed matter physics and beyond.

References

- [1] A. Altland and B.D. Simons *Condensed matter field theory*, CUP, Cambridge (2006).
- [2] P.M. Chaikin and T.C. Lubensky, *Principles of Condensed Matter Physics*, CUP, Cambridge (1995).
- [3] G.F.R. Ellis, *Top-down causation and emergence: some comments on mechanisms* Interface Focus **2**, 126 (2012).
- [4] S.J. Blundell *Emergence, causation and storytelling: condensed matter physics and the limitations of the human mind* arXiv:1604.06845 (2016).
- [5] J.J. Binney, N.J. Dowrick, A.J. Fisher, M.E.J. Newman *The theory of critical phenomena*, OUP, Oxford (1992).
- [6] T. Lancaster and S.J. Blundell *Quantum Field Theory for the Gifted Amateur* OUP, Oxford (2014).
- [7] P.W. Anderson *Basic notions of condensed matter physics*, Westview, Colorado (1984).
- [8] D. Bohm and D. Pines, *A Collective Description of Electron Interactions: II. Collective Individual Particle Aspects of the Interactions*, Phys. Rev. **85**, 228 (1952).
- [9] P. A. M. Dirac *Quantum Mechanics of Many-Electron Systems*’ Proceedings of the Royal Society of London. Series A, Containing Papers of a Mathematical and Physical Character **123**, 714 (1929).

- [10] D. Calvania, A. Cuccolia, N.I. Gidopoulos and P. Verrucchia *Parametric representation of open quantum systems and cross-over from quantum to classical environment*, Proc, Nat, Acad. Sci. USA **110**, 6748 (2013).
- [11] P. Hohenberg and W. Kohn. *Inhomogeneous Electron Gas* Phys. Rev., **136**, 864B (1964).
- [12] W. Kohn and L. J. Sham *Self-Consistent Equations Including Exchange and Correlation Effects* Phys. Rev. **140**, 1133A (1965).
- [13] Segall, M. D.; Lindan, P. J. D.; Probert, M. J.; Pickard, C. J.; Hasnip, P. J.; Clark, S. J.; Payne, M. C. *First-principles simulation: ideas, illustrations and the CASTEP code*, J. Phys.: Condens. Matter, **14**, 2717 (2002).
- [14] Clark, S. J.; Segall, M. D.; Pickard, C. J.; Hasnip, P. J.; Probert, M. J.; Refson, K.; Payne, M. C. *First principles methods using CASTEP*, Zeitschrift fuer Kristallographie, **220**, 567 (2005).
- [15] Kurt Lejaeghere *et al.* *Reproducibility in density functional theory calculations of solids*, Science **351**, 25 (2016).